

Propane, 2-methyl-2-nitro-  
594-70-7 | DTXSID0060488

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 37.4 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 6.01e-01

**Confidence level:** 6.53e-01

## Nearest Neighbors from the Training Set

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Benzene

**Measured:** 56.2

**Predicted:** 50.5

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Toluene

**Measured:** 117

**Predicted:** 87.4

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Resorcinol

**Measured:** 9.55

**Predicted:** 28.3

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Phenol

**Measured:** 26.9

**Predicted:** 57.3

Image not found

Pyridine

**Measured:** 39.8

**Predicted:** 20.1